

## Compound Selection Criteria

Compounds are selected for inclusion in the MLSMR collection based on the following criteria:

- a. Samples are at least 90% pure; each sample is tested for identity and purity.
- b. At least 10 mg of each sample is available from the supplier.
- c. Compounds have an acceptable range of physicochemical properties, including calculated water solubility, to allow good performance in HTS assays
- d. Compounds exclude reactive functional groups or moieties known to interfere with HTS.
- e. Compounds contribute to the diversity of their class. MLSMR clusters as many as four close analogs around each diverse compound to provide some Structure Activity Relationship (SAR) data for screening hits.
- f. Additional information on the compound selection strategy and the MLSMR compound collection can be found at the MLSMR website ([link](#)).

Following the selections of which compounds to include, the MLSMR undertakes all activities necessary to acquire sufficient quantities (typically 5-30 mg) of compounds selected for inclusion in the Small Molecule Repository collection. The collection will expand on a continuing basis and evolve over time- based on the biological activity/utility of the compounds as assessed by screening.